

Curriculum Vitae

Eric J. Cockayne
Birthdate: June 20, 1966
Citizenship: U.S.A.
Telephone: (301) 975-4347
Fax: (301) 975-5334
E-mail: cockayne@nist.gov

Ceramics Division
National Institute of Standards and Technology
100 Bureau Dr. Stop 8520
Gaithersburg, MD 20899-8520

Education

B.S. State University of New York at Buffalo, Physics (summa cum laude), May 1988
Ph.D. Cornell University, Physics, January 1994
Thesis topic: Quasicrystals and Instabilities of the 2D Wigner Crystal
Thesis advisor: Professor Veit Elser

Professional Employment

5/87-8/88: Undergraduate research assistant, SUNY at Buffalo. Supervisor: Professor Michael Ram.

8/88-9/93: NSF fellow and graduate research assistant in the Laboratory of Atomic and Solid State Physics, Cornell University. Supervisor: Professor Veit Elser.

9/93-9/95: Chateaubriand fellow and postdoctoral research associate at Laboratoire de Physique des Solides, Université de Paris-Sud, France. Supervisor: Dr. Françoise Dénoyer.

10/95-8/98: Postdoctoral research associate in the Department of Applied Physics, Yale University. Supervisor: Professor Karin Rabe.

8/98-8/00: NRC fellow and postdoctoral research associate in the Ceramics Division, NIST. Supervisor: Dr. Terrell A. Vanderah

9/00-8/01 Research associate in the Physics Department, Catholic University of America, and Guest Researcher in the Ceramics Division, NIST.

8/01-present Research scientist in the Ceramics Division, NIST. Supervisor: Dr. Terrell A. Vanderah

Scholarships and Fellowships

SUNY at Buffalo (1984-1988)

National Merit Scholarship (1984-1985)

SUNY at Buffalo Presidential Honors Scholarship (1984-1988)

Cornell University (1988-1993)

NSF Fellowship (1988-1991)

Cornell University A.D. White Fellowship (1988-1991)

Université Paris-Sud (1993-1995)

Chateaubriand Fellowship (French Government) (1993-1995)

NIST (1998-2000)

NRC Postdoctoral Fellowship (1998-2000)

Research Interests

Structure of ferroelectric solid solutions; lattice dynamics of ferroelectrics; ab initio modeling of ferroelectric phase transitions; piezoelectricity in mixed ferroelectrics; dielectric properties of complex oxides.

Quasicrystal structure; quasicrystal tiling theory; the quasicrystal sphere packing problem.

Personal References

Dr. Benjamin P. Burton
Ceramics Division
NIST
100 Bureau Dr. Stop 8520
Gaithersburg, MD 20899-8520
(301) 975-6043
bburton@nist.gov

Professor Karin M. Rabe
Department of Physics and Astronomy
Rutgers University
136 Frelinghuysen Road
Piscataway, NJ 08854-8019
(732) 445-4186
rabe@physics.rutgers.edu

Professor Veit Elser
Department of Physics
Cornell University
Ithaca, NY 14853-2501
(607) 255-2340
veit@msc.cornell.edu

Professor Mike Widom
Department of Physics
Carnegie Mellon University
Pittsburgh, PA 15217
(412) 268-7645
widom@andrew.cmu.edu

Dr. Françoise Dénoyer
Laboratoire de Physique des Solides
Bâtiment 510
Université Paris-Sud
91405 Orsay Cedex
France
(011-33) 1-69-41-60-60
denoyer@lps.u-psud.fr

Publications

Eric J. Cockayne

1. Eric Cockayne, "First principles calculations of the dielectric properties of perovskite-type materials", submitted to Journal of the European Ceramic Society.
2. Umesh V. Waghmare, Eric Cockayne, and Benjamin P. Burton, "Ferroelectric phase transitions in nano-scale chemically ordered $\text{PbSc}_{0.5}\text{Nb}_{0.5}\text{O}_3$ using a first-principles model Hamiltonian", submitted to Ferroelectrics.
3. L. Jastrabik, M. Savinov, S. Kapphan, V. Trepakov, E. Cockayne, B. P. Burton, and S. A. Prosandeev, "Properties of $\text{K}_{1-x}\text{Li}_x\text{TaO}_3$ Solid Solutions: First Principles Computations and Experiments", Japanese Journal of Applied Physics (to appear).
4. V. Zelezny, Eric Cockayne, J. Petzelt, M. F. Limanov, D. Usvyat, V.V. Lemanov, and A.A. Volkov, "Temperature dependence of infrared-active phonons in CaTiO_3 : a combined spectroscopic and first-principles study", Physical Review B (to appear).
5. Serguei Prosandeev, Eric Cockayne, and Benjamin Burton, "First principles studies of KNbO_3 , KTaO_3 , and LiTaO_3 solid solutions", in "Fundamental Physics of Ferroelectrics 2002" (AIP Conference Proceedings 626), edited by Ronald E. Cohen (American Institute of Physics, Woodbury, NY) (2002), 64-73.
6. B. P. Burton and E. Cockayne, "Unexpected ground state structures in relaxor ferroelectrics", Ferroelectrics **270**, 1359 (2002).
7. K. Leung, Eric Cockayne, and A. F. Wright, "Effective Hamiltonian Study of PZT 95/5", Physical Review B **65**, article 214111 (13 pages) (2002).
8. M. Mihalkovič, I. Al-Lehyani, E. Cockayne, C. L. Henley, N. Moghadam, J. A. Moriarty, Y. Wang, and M. Widom, "Total-energy based structure prediction for decagonal Al-Ni-Co", Physical Review B **65**, article 104205 (6 pages) (2002).
9. Eric Cockayne, Benjamin P. Burton, and Laurent Bellaiche, "Temperature dependent behavior of $\text{PbSc}_{1/2}\text{Nb}_{1/2}\text{O}_3$ from first principles", in *Fundamental Physics of Ferroelectrics 2001* (AIP Conference Proceedings 582), edited by Henry Krakauer (American Institute of Physics, Woodbury, NY) (2001), 191-200.
10. B.P. Burton and E. Cockayne, "Prediction of the $[\text{Na}_{1/2}\text{Bi}_{1/2}]\text{TiO}_3$ ground state", in *Fundamental Physics of Ferroelectrics 2001* (AIP Conference Proceedings 582), edited by Henry Krakauer (American Institute of Physics, Woodbury, NY) (2001), 82-90.
11. Eric Cockayne, "Comparative dielectric response of CaTiO_3 and $\text{CaAl}_{1/2}\text{Nb}_{1/2}\text{O}_3$ from first principles", J. Appl. Phys. **90**, 1459-1468 (2001).
12. Eric Cockayne, "Generation of quasicrystals via a single cluster", Mater. Sci. Engin. A **294**, 224-227 (2000).
13. Michael Widom, Ibrahim Al-Lehyani, Yang Wang, and Eric Cockayne, "Ab initio energetics of transition metal ordering in decagonal Al-Cu-Co", Mater. Sci. Engin. A **294**, 295-298 (2000).
14. Eric Cockayne and Benjamin P. Burton, "Phonons and Static Dielectric Constant in CaTiO_3 from first principles", Phys. Rev. B **62**, 3735-3743 (2000).

15. Eric Cockayne and Karin M. Rabe, "Pressure Dependence of instabilities in perovskite PbZrO_3 ", J. Phys. Chem. Solids **61**, 305-308 (2000).
16. Eric Cockayne, "Random tiling models for quasicrystals", chapter in *From Quasicrystals to More Complex Systems*, F. Axel, F. Dénoyer and J. P. Gazeau, editors, (EDP Sciences, Les Ulis (France)/Springer-Verlag, Berlin) (2000), 115-143.
17. Bruce Ravel, Eric Cockayne, Mark Newville, and Karin M. Rabe, "A combined EXAFS and First-Principles Study of $\text{Pb}_{1-x}\text{Ge}_x\text{Te}$ ", Phys. Rev. B **60**, 14632-14642 (1999).
18. B. P. Burton and E. Cockayne, "Why $\text{Pb}(B, B')\text{O}_3$ perovskites disorder at lower temperatures than $\text{Ba}(B, B')\text{O}_3$ perovskites", Phys. Rev. B **60**, R12542-R12545 (1999).
19. Eric Cockayne and Marek Mihalkovič, "Stable Quasiperiodic Sphere Packing", Phil. Mag. Lett. **79**, 441-448 (1999).
20. Ph. Ghosez, E. Cockayne, U. V. Waghmare and K. M. Rabe, "Lattice dynamics of BaTiO_3 , PbTiO_3 and PbZrO_3 : a comparative first-principles study", Phys. Rev. B **60**, 836-843 (1999).
21. Bruce Ravel, Eric Cockayne, and Karin M. Rabe, "The local structure of ferroelectric $\text{Pb}_{1-x}\text{Ge}_x\text{Te}$ ", J. Synchrotron Rad. **6**, 567-569 (1999).
22. Eric Cockayne and Mike Widom, "Ternary model of an AlCuCo decagonal quasicrystal", Phys. Rev. Lett. **81**, 598-601 (1998).
23. Eric Cockayne and Karin M. Rabe, "Configuration Dependence of Physical Properties of a Ferroelectric Solid Solution", in *First Principles Calculations for Ferroelectrics: Fifth Williamsburg Workshop* (AIP Conference Proceedings 436), edited by R. E. Cohen, (American Institute of Physics, Woodbury, NY) (1998), 71-80.
24. K. M. Rabe and E. Cockayne, "Temperature-dependent dielectric and piezoelectric response of ferroelectrics from first principles", in *First Principles Calculations for Ferroelectrics: Fifth Williamsburg Workshop* (AIP Conference Proceedings 436), edited by R. E. Cohen, (American Institute of Physics, Woodbury, NY) (1998), 61-70.
25. Eric Cockayne and Karin M. Rabe, "Enhancement of piezoelectricity in a mixed ferroelectric", Phys. Rev. B **57**, R13973-R13976 (1998).
26. Eric Cockayne and Mike Widom, "Structure and phason energetics of AlCo decagonal phases", Phil. Mag. A **77** 593-619 (1998).
27. Eric Cockayne and Karin M. Rabe, "Ab initio study of the ferroelectric transition in cubic Pb_3GeTe_4 ", Phys. Rev. B **56**, 7947-7961 (1997).
28. Eric Cockayne and Mike Widom, "Structure and excitations of orthorhombic Al_3Co ", in *New Horizons in Quasicrystals: Research and Applications*, eds. A.I. Goldman, D.J. Sordet, P.A. Thiel and J.M. Dubois (World Scientific, 1997) pp. 21-28.
29. Mike Widom and Eric Cockayne, "Atomic correlations in AlCo decagonal phases", Physica A **232**, 713-722 (1996).
30. M. Widom and E. Cockayne, "Structure and phason energetics of AlCo decagonal phases", in *Proceedings of the 5th International Conference on Quasicrystals*, C. Janot and R. Mosseri, eds., World Scientific, Singapore (1995), 343-350.

31. Eric Cockayne, "The quasicrystalline sphere packing problem", in *Proceedings of the 5th International Conference on Quasicrystals*, C. Janot and R. Mosseri, eds., World Scientific, Singapore (1995), 224- 227.
32. Eric Cockayne, "Dense quasiperiodic decagonal disc packing", *Phys. Rev. B* **51**, 14958-14961 (1995).
33. Eric Cockayne, Mike Widom, Pascale Launois, Manfred Fettweis and Françoise Dénoyer, "Aluminum-cobalt pair potentials and the structure of decagonal Al-Co-Cu", in *Aperiodic '94*, G. Chapuis and W. Paciorek, eds., World Scientific, Singapore (1995).
34. Jacques Peyrière, Eric Cockayne and Françoise Axel, "Line-shape analysis of high resolution x-ray diffraction spectra of finite size Thue-Morse GaAs-AlAs multilayer heterostructures", *J. de Physique I (France)* **5**, 111-127 (1995).
35. Eric Cockayne, "Atomistic octagonal random-tiling model", *J. Phys. A: Math. Gen.* **27**, 6107-6119 (1994).
36. Eric Cockayne, "Non-connected atomic surfaces for the quasicrystalline sphere packing problem", *Phys. Rev. B* **49**, 5896-5910 (1994).
37. R.C. Haddon, E. Cockayne and V. Elser, "Calculated magnetic susceptibilities of C₆₀, C₇₀ and C₈₄ and their ions", *Synth. Metals* **59**, 369-376 (1993).
38. David P. DiVincenzo, William Krakow, Peter A. Bancel, Eric Cockayne and Veit Elser, "An atomic model of Al-Cu-Fe and its comparison with high-resolution electron microscope images", *J. Noncryst. Sol.* **153**, 145-149 (1993).
39. Eric Cockayne, Rob Phillips, X.B. Kan, S.C. Moss, J.L. Robertson, T. Ishimasa and M. Mori, "Use of periodic approximants in the structure refinement of icosahedral AlCuFe", *J. Noncryst. Sol.* **153**, 140-144 (1993).
40. William Krakow, David P. DiVincenzo, Peter A. Bancel, Eric Cockayne and Veit Elser, "High resolution electron microscopy of Al-Cu-Fe quasicrystals: atomic structure and modeling", *J. Mater. Res.* **8**, 24-37 (1993).
41. Eric Cockayne, "Comment on 'Stability of the Wigner electron crystal on the perovskite lattice'", *J. Phys.: Cond. Matter* **3**, 8757-8758 (1991).
42. R.C. Haddon, L.F. Schneemeyer, J.V. Waszczak, S.H. Glarum, R. Tycko, G. Dabbagh, A.R. Kortan, A.J. Muller, A.M. Muzsca, M.J. Rosseinsky, S.M. Zahurak, A.V. Makhija, F.A. Thiel, K. Raghavachari, E. Cockayne and V. Elser, "Experimental and theoretical determination of the magnetic susceptibility of C₆₀ and C₇₀", *Nature* **350**, 46-47 (1991).
43. Eric Cockayne and Veit Elser, "Energetics of point defects in the two-dimensional Wigner crystal", *Phys. Rev. B* **43**, 623-629 (1991).